ADVANCED MATERIALS

Supporting Information

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Photoalignment and Surface-Relief-Grating Formation are Efficiently Combined in Low-Molecular-Weight Halogen-Bonded Complexes

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Submitted to ADVANCED FUNCTIONAL MATERIALS

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Supporting Information

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S1. Single crystal X-Ray diffraction analysis.

Crystallographic data of 3. Chemical formula: $C_{28}H_{23}F_4ION_4$; M_r = 634.40; monoclinic, $P2_1/n$; crystal color: dark-red; shape: wedge; dimensions: 0.12×0.25×0.32 mm^3, a = 10.2984(15), b = 8.8606(12), c = 28.157(4) Å, β = 94.345(12)°, Z = 4, d_{calc} = 1.645 g cm^{-3}, μ(Mo-$K\alpha$) = 1.309 mm^{-1}, temperature 103(2) K. Crystallographic data have been collected on a Bruker Smart APEX-II CCD diffractometer, equipped with a Bruker KRIOFLEX low temperature device; data collection range 2.06 < θ < 36.23 ° (completeness = 1.00 for θ < 32.00 °), $\theta/2\theta$ scan mode, 97266 collected reflections, 10581 independent, 9057 with $I > 2\sigma(I)$, multi-scan absorption correction: 0.6606 ≤ T ≤ 0.7471, R_{ave} = 0.0297. The structure was solved by *SIR2002*[S1], and refined by *SHELXL*[S2]. Anisotropic heavy atoms, isotropic hydrogen atoms; H atoms were refined with soft restraints, imposing similar distance on chemically equivalent C-H distances and on H-C-H methyl angles; 412 parameter refined, 178 restraints; final disagreement factors based on all (and 'observed') independent reflections R = 0.0511 (0.0415) and wR = 0.0991(0.0947), GOF = 1.134.

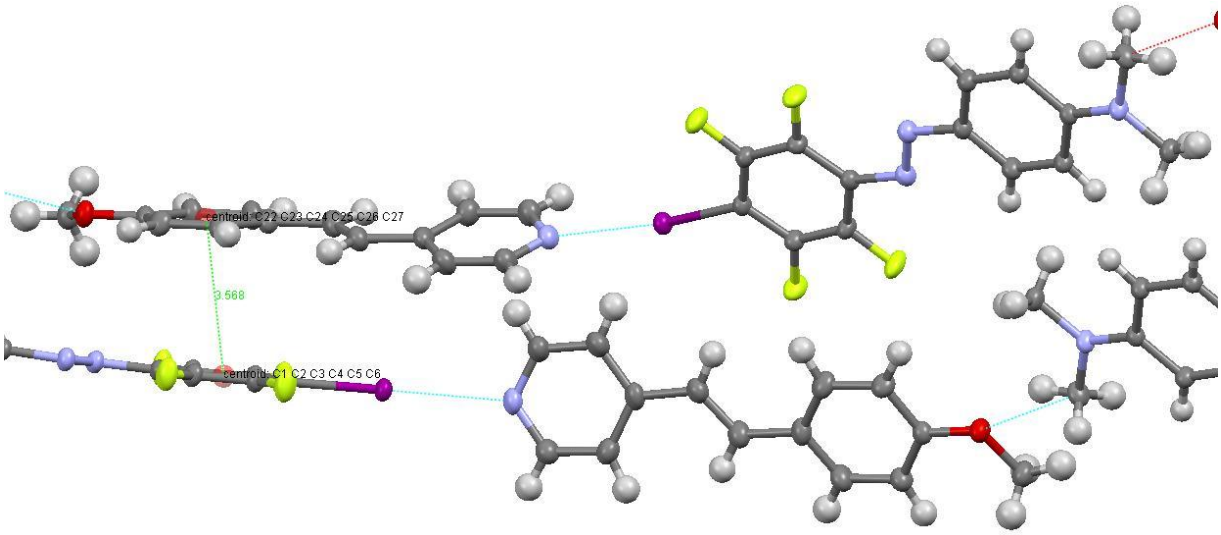

Figure S1: Crystal packing of the supramolecular complex **3** formed upon XB driven self-assembly of **1** and **2**. Ball and stick model. Colors are as follows: C, gray; H, light gray; N, sky blue; F, yellowish green, I, magenta.

S2. X-Ray powder diffraction analysis

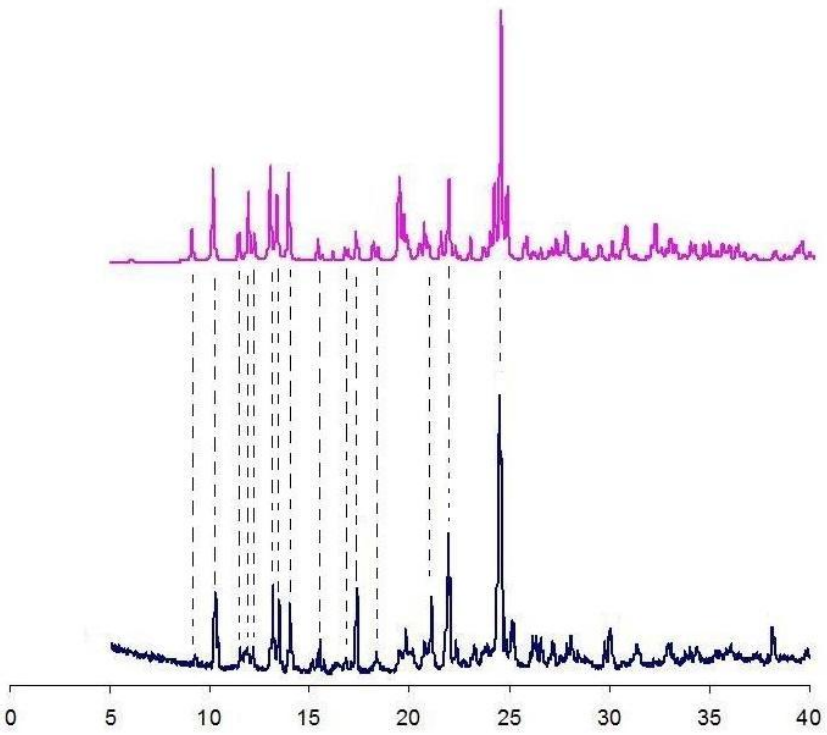

Figure S2: Simulated from single crystal data (top) and experimental (bottom) XRPD patterns of **3**

[S1] M.C. Burla, M. Camalli, B. Carrozzini, G.L. Cascarano, C. Giacovazzo, G. Polidori, R. Spagna, *J. Appl. Crystallogr*. **2003**, *36*, 1103.

[S2] G. M. Sheldrick, *Acta Crystallogr. A*, **2008**, *64*, 112.